Granular Flow: Friction and the Dilatancy Transition

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Molecular-dynamics simulations of noncohesive granular assemblies under shear are described. At low shear rate $\dot{\gamma}$, the assembly is unstable to uniform motion and exhibits stick-slip dynamics involving periodic dilatancy transitions and gravitational compactification. Steady-state motion occurs at larger $\dot{\gamma}$ where 6–12 layers of grains flow over a compact, static assembly. A phase boundary, characterized by a discontinuity in $\dot{\gamma}$ and an enhanced normal stress, separates the static and flowing regions. In the steady-state regime, dilatancy leads to a shear stress that is independent of $\dot{\gamma}$.

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The physics of noncohesive granular assemblies, such as sand, is intriguing and has been a subject of great interest for well over two centuries [1–4]. On one hand, granular assemblies exhibit solidlike behavior: They can resist shear by undergoing plastic deformation. Yet, anyone who has watched an hourglass or an avalanche down a sandpile knows that granular assemblies can also flow, much like a fluid.

Our knowledge of granular assemblies is essentially confined to two extremes. The compact, solidlike state is well described by theories of soil mechanics [5], whereas the low-volume-fraction, high-shear-rate flow can be treated by drawing on the ideas of kinetic theory [6]. What has remained elusive, however, is the underlying dynamics of the low-shear-rate or quasistatic regime, where the assembly undergoes transitions between static and flowing states [4,6–8]. Understanding the latter is crucial to an understanding of many geophysical phenomena such as earthquakes and rockslides. It is also relevant to important industrial problems, including the handling of powders, and the design of coal slurries and fluidized bed reactors.

The fundamental difficulties impeding our understanding lay with the very properties of granular media that make it so interesting to study in the first place: dilatancy, bistability, arching, segregation, and thixotropy. These properties conspire to create substantial hysteresis and instability, limiting experimental control and reproducibility [3,6–9]. Analytical treatments are also difficult because the boundary conditions and velocity distribution functions are poorly understood, and microstructure induces complex correlations among grains [4,6,7].

In this paper, we describe molecular-dynamics simulations of granular flow which reproduce many of the phenomena observed experimentally [8,9]. We find a simple relationship between friction and shear rate $\dot{\gamma}$ in granular assemblies at constant normal stress. For $\dot{\gamma}$ greater than a certain critical value $\dot{\gamma}_c$, the frictional force or shear stress is a constant. Below $\dot{\gamma}_c$, the system is unstable to gravitational compactification and only static solutions exist. This gives rise to a shear-induced, phase boundary between static and flowing states. When a portion of the assembly is forced to flow with an average shear rate less than $\dot{\gamma}_c$, a generic stick-slip motion is observed. The origin of this oscillatory motion is periodic dilatancy transitions and gravitational compactification.

The simulations were two dimensional and performed in Couette and chute geometries (Fig. 1). In the Couette cell, disklike grains of diameter d and mass m were confined in the $\hat{\mathbf{y}}$ direction by two walls, each composed of a rigid layer of grains of diameter d_w [Fig. 1(a)]. Shear was induced across the cell by translating the top wall at constant velocity $U\hat{\mathbf{x}}$. Rather than fixing the separation of the two walls, a constant load per unit length P_{ext} was exerted on the top wall. This allowed for dilation. In the chute geometry, the top wall was removed, creating a free-boundary condition [Fig. 1(c)]. Shear was induced by tilting the bottom wall at an angle $(90° - \theta)$ with respect to the gravitational field $\mathbf{g}$. In both geometries, periodic boundary conditions were imposed along the x axis.

A number of models have been developed to simulate inelastic collisions between cohesiveless grains [10,11]. We used a variation of one developed by Haff and

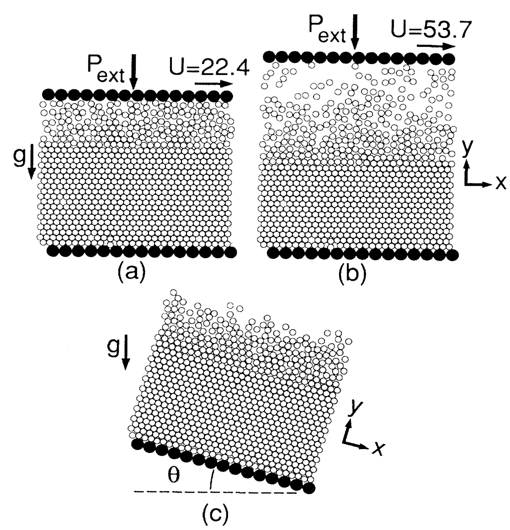

FIG. 1. Instantaneous configurations during steady-state flow of 750 grains in (a),(b) Couette and (c) chute geometries with $e=0.92$, $d_w/d=2$, $P_{\text{ext}}=24mgd^{-1}$, and $\theta=15°$. The systems span $30d$ in the x direction and have walls with mass $30m$. The units of U in (a) and (b) are $(gd)^{1/2}$.

Werner [11] to study the mechanical sorting of sand. The model is advantageous because it simulates the basic features of the collisions with a continuous potential that is easily vectorized. The grains are modeled as rubber disks with both translational and rotational degrees of freedom. Two grains undergo an inelastic collision whenever the distance separating them is less than the sum of their radii, $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|<d$. During the collision the ith grain feels a contact force that has both normal and shear components,

$$\mathbf{F}_{ij}(t)=\{k_n(d-r_{ij})-\gamma_n m(\dot{\mathbf{r}}_{ij}\cdot\hat{\mathbf{n}})/2\}\hat{\mathbf{n}} + \{\min(-\gamma_s m v_{\mathrm{rel}}/2,\mu|\mathbf{F}\cdot\hat{\mathbf{n}}|)\}\hat{\mathbf{s}}\,, \quad (1)$$

where $v_{\mathrm{rel}}=\dot{\mathbf{r}}_{ij}\cdot\hat{\mathbf{s}}+d(\dot{\phi}_i+\dot{\phi}_j)/2$, $\hat{\mathbf{n}}=(\mathbf{r}_{ij}\cdot\hat{\mathbf{x}},\mathbf{r}_{ij}\cdot\hat{\mathbf{y}})/r_{ij}$, $\hat{\mathbf{s}}=(\mathbf{r}_{ij}\cdot\hat{\mathbf{y}},-\mathbf{r}_{ij}\cdot\hat{\mathbf{x}})/r_{ij}$, and $\dot{\phi}_i$ is the angular velocity of the ith grain. The strength of the collision is characterized by k_n, the elastic constant for deformations along the collision normal. γ_n and γ_s are damping constants in the normal and shear directions. In order to satisfy the Coulomb proportionality between shear and normal stresses in fully developed planar shear [1,5,6], the shear force in Eq. (1) is limited by the product of the frictional coefficient μ and the normal force $|\mathbf{F}\cdot\hat{\mathbf{n}}|$. In our simulations $\mu=0.5$ [12].

Nonzero γ_n and γ_s ensure that collisions between grains are inelastic. The amount of energy lost is characterized by the coefficient of restitution, e. For collisions governed by Eq. (1), there are separate coefficients for the shear and normal directions: $e_n=\exp(-\gamma_n t_{\mathrm{col}}/2)$ and $e_s=\exp(-\gamma_s t_{\mathrm{col}})$, where $t_{\mathrm{col}}=\pi(2k_n/m-\gamma_n^2/4)^{1/2}$. We set $\gamma_n=2\gamma_s$ so that $e_n=e_s$. Note that there is considerable freedom in choosing a value for k_n. In general, k_n should be large to prevent the grains from interpenetrating. However, it should not be so large that it requires an unreasonably small simulation time step Δt. An accurate simulation typically requires $\Delta t \sim t_{\mathrm{col}}/50$. In our study, we set $k_n=2\times10^5 mgd^{-1}$, and used $\gamma_n=33.5(g/d)^{1/2}$ for $e=0.92$, and $\gamma_n=80.5(g/d)^{1/2}$ for $e=0.82$. The equations of motion were integrated using a third-order, Gear predictor-corrector scheme with $\Delta t=1.12\times10^{-4}(d/g)^{1/2}$.

An important property of granular assemblies under constant load is their tendency to dilate with increasing shear [2,3]. This is clearly evident in our simulations. In Figs. 1(a) and 1(b), we show instantaneous configurations of 750 grains in Couette cells with different U. Notice that the wall separation increases rapidly with U. As in experiments, we find that only a small portion of the assembly actually contributes to the flow [9]. For a broad range of parameters, this typically amounts to 6–12 layers of grains.

Dilatancy has important ramifications for the shape of the shear stress curve characterizing granular flow. In Fig. 2, the shear stress P_{xy} is plotted as a function of U for systems with different e. Notice that the curves are flat at large U, in sharp contrast with the $\dot{\gamma}^2$ dependence expected in the absence of dilation [3,4,7]. A similar result has been reported by Johnson and Jackson [6], who used a kinetic theory approach to study partial flow in shear cells. This suggests that constant P_{xy} may be a generic feature of granular flow at large $\dot{\gamma}$ under constant load.

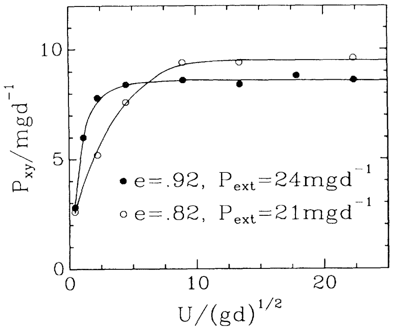

FIG. 2. Shear stress vs U for systems with $d_w/d=2$, and the indicated values of e and P_{ext}. The solid lines are merely visual guides.

The granular assembly is more compact at small U. In this regime, dilatancy is confined to a small region near the top wall, where layers of grains slide over each other. As shown in Fig. 2, this layered microstructure coincides with a drastic reduction in friction [13]. This is consistent with previous experiments and simulations which showed that the effective coefficient of friction at large volume fraction ν decreases with increasing ν [4]. Such behavior is particularly interesting in light of experiments at small $\dot{\gamma}$ where instabilities, such as stick-slip motion, are observed [3,9]. Normally, these instabilities are assumed to be *dynamical* in origin: That is, the frictional force decreases with increasing velocity [7,14]. If in fact P_{xy} is a monotonically increasing function of U, as the simulations suggest, what is the origin of these instabilities?

Recently, a similar frictional dependence at small U was observed in studies of boundary lubrication [15]. These systems also exhibited stick-slip dynamics. In this case, it was shown that the origin of the oscillatory motion was a thermodynamic instability, not a *dynamical* one due to $dP_{xy}/dU<0$. This raises the question of whether an analogous instability exists in the granular systems.

To explore this possibility, we relaxed the constant-U constraint on the top wall by pulling it with a spring connected to a stage translating at constant velocity $U_{\mathrm{sp}}\hat{\mathbf{x}}$ [16]. For values of U_{sp} in the flat region of the shear stress curve, the wall translated uniformly. However, for U_{sp} in the decreasing region, the system was unstable, and the top wall exhibited stick-slip dynamics, analogous to that observed in boundary lubrication [15]. The basic features of the stick-slip motion are shown in Fig. 3 for a single U_{sp} and are described at length elsewhere [15]. The important feature to note in this case is that the top plate moves vertically when sliding occurs and collapses when the static period returns [Fig. 3(c)]. This suggests

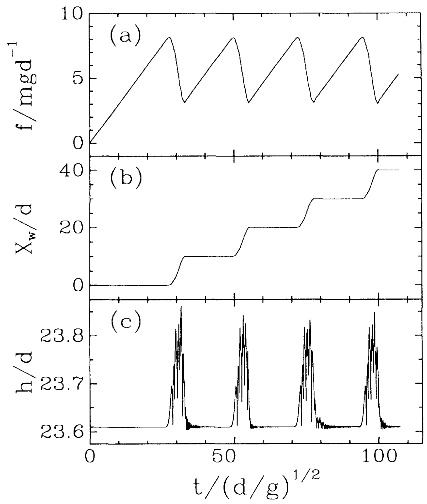

FIG. 3. Time profiles of (a) the force per unit length exerted on the top wall f, (b) the wall displacement X_w, and (c) the wall spacing h during stick-slip motion for a system with $U_{sp}=0.45(gd)^{1/2}$, $P_{ext}=21mgd^{-1}$, $e=0.82$, and $d_w/d=2$. The spring which couples the wall and translation stage has stiffness $20mgd^{-1}$.

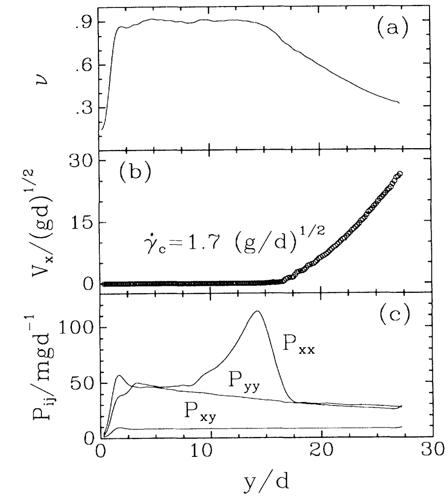

FIG. 4. Profiles normal to the wall of (a) volume fraction ν, (b) velocity in the shear direction V_x, and (c) components of the microscopic stress tensor for a system with $U=33.5(gd)^{1/2}$, $P_{ext}=24mgd^{-1}$, $e=0.92$, and $d_w/d=2$. The bottom wall is located at $y=0$.

that the origin of stick-slip motion in granular assemblies is periodic dilatancy transitions and gravitational compactification, not a frictional force that decreases with increasing U as previously assumed [7].

So far we have discussed properties of granular flow that are strongly dependent on boundary conditions at the walls. To generalize our study for arbitrary geometries, we now focus on the behavior away from the walls. In Fig. 4 we show profiles of the volume fraction ν, the velocity in the shear direction V_x, and components of the microscopic stress tensor P, for steady-state partial flow. These quantities were time averaged within bins spanning the length of the simulation cell for a period of $72(d/g)^{1/2}$. Because the system is highly layered, ν and P were smoothed by a Gaussian with a standard deviation of $0.5d$.

The most striking feature of the velocity profile [Fig. 4(b)] is that the local shear rate, $\dot{\gamma}=\partial V_x/\partial y$, does not go continuously to zero between the flowing and static regions. Instead, there is a sharp discontinuity at $\dot{\gamma}=\dot{\gamma}_c$. For the system shown in Fig. 4, $\dot{\gamma}_c\simeq 1.7(g/d)^{1/2}$. In general, we find that $\dot{\gamma}_c$ increases with increasing P_{ext} and decreasing e. This shear-induced phase boundary is due to a gravitational instability. For given normal and shear stresses, there is a critical shear rate $\dot{\gamma}_c$ below which the granular assembly is unstable to gravitational compactification. The existence of such a critical shear rate was predicted in earlier analytical studies [3,6]. Note that the sharp cutoff in $\dot{\gamma}$, coupled with well-defined layering in the shear direction, enhances the normal stress component P_{xx} in the vicinity of the phase boundary [Fig. 4(c)]. In polydisperse assemblies, packing of the grains at the boundary is less ordered and this enhanced stress is not observed [17].

The phase boundary is particularly sharp for assemblies of monodisperse disks, because they easily form triangular arrays which have a static yield that is substantially greater than dynamic yield. This static yield is easily estimated assuming a Coulomb proportionality between normal and shear stresses at the phase boundary, $P_{xy}=P_{yy}\tan\theta_m$, where θ_m is the friction angle at initial yield [5,6]. We computed θ_m using a chute geometry [Fig. 1(c)]. The inclination angle of a static triangular array of grains was slowly increased until flow initiated at the free surface. The latter occurred at $\theta_m=32.0°\pm0.5°$, independent of e. The dynamic yield at the phase boundary is $P_{xy}=P_{yy}\tan\theta_r$, where θ_r is the friction angle at which motion ceases, also known as the angle of repose. Using the components of the microscopic stress tensor at the phase boundary [18], we found $\theta_r\simeq 15°$ for $e=0.92$.

We are now in a position to map out the frictional force as a function of $\dot{\gamma}$ for a granular assembly at fixed normal stress, independent of the details at the bounding walls. For a large number of simulations with different U and P_{ext}, we extracted P_{xy} and $\dot{\gamma}$ at various P_{yy}. Results are shown in Fig. 5 for $e=0.92$. Note that each stress curve is characterized by a critical shear rate $\dot{\gamma}_c$. For $\dot{\gamma}>\dot{\gamma}_c$, the shear stress is a constant. Below $\dot{\gamma}_c$, the system is unable to support the shear against gravitational compactification, and there is a discontinuous jump to $\dot{\gamma}=0$. Simulations of polydisperse assemblies indicate that both P_{xy} at yield and $\dot{\gamma}_c$ decrease [17]. However, the qualitative features of the stress curves remain the same.

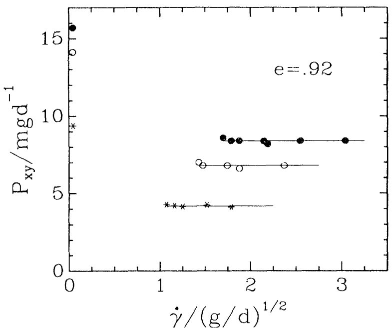

FIG. 5. Shear stress vs $\dot{\gamma}$ measured in various systems with $e=0.92$ at $P_{yy}=31mgd^{-1}$ (solid circles), $P_{yy}=26mgd^{-1}$ (open circles), and $P_{yy}=16mgd^{-1}$ (stars). The shear stresses at static yield were obtained using the Coulomb relation $P_{xy}=P_{yy}\times\tan\theta_m$. θ_m was measured in a chute geometry with $d_w/d=1$.

It is interesting to note that the stick-slip motion, which arises when the walls are used to drive a portion of the system in the unstable regime ($\dot{\gamma}<\dot{\gamma}_c$), is remarkably similar to that observed in earlier boundary lubrication studies [15]. As $\dot{\gamma}$ approaches $\dot{\gamma}_c$, the stick-slip motion becomes increasingly irregular because the system does not have enough time to fully order. In addition to fluctuations in the yield stress, this disorder causes intermittent periods of uniform sliding. Whether or not there is universality in this transition is an intriguing open issue. Regardless, the transition has fundamental implications. Because the yield stress decreases with increasing disorder, temporal or spatial averaging of the stick-slip produces an *apparent* frictional force that decreases with increasing $\dot{\gamma}$ [15]. Similar frictional curves have been used to model many of the salient features of earthquakes [19] and sandpile dynamics [7].

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